Macromolecular Symposia 2004 vol.217, pages 267-272

Polymer chain dynamics predicted by n-renormalized rouse models: Numerical studies

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Abstract

Features of the renormalized and twice renormalized Rouse models were examined numerically. Based on numerical evaluations of the generalized Langevin equation in renormalization approaches, nonexponential normal mode autocorrelation functions were derived, that can be described over two orders of magnitude by stretched exponential functions. The mode number dependence of the stretching parameter was evaluated. The consequences of the nonexponential correlation functions on dynamical properties are discussed. As a basis for predictions for the behavior of diffusion and spin-lattice relaxation dispersion, the time dependence of the mean-squared segment displacement and of the autocorrelation function of the segment tangential vector, respectively, were obtained taking into account finite chain lengths.

http://dx.doi.org/10.1002/masy.200451321

Keywords

Generalized Langevin equation, Relaxation, Renormalized Rouse model, Segment diffusion, Theory